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# IUCLID

# Data Set

| | | |
|---|---|---|
| **Existing Chemical** | : | ID: 108419-35-8 |
| **CAS No.** | : | 108419-35-8 |
| **TSCA Name** | : | Acetic acid, C11-14-branched alkyl esters, C13-rich |
| **Molecular Formula** | : | Unspecified |
| | | |
| **Producer related part** | | |
| **Company** | : | ExxonMobil Biomedical Sciences Inc. |
| **Creation date** | : | 07.12.2000 |
| | | |
| **Substance related part** | | |
| **Company** | : | ExxonMobil Biomedical Sciences Inc. |
| **Creation date** | : | 07.12.2000 |
| | | |
| **Status** | : | |
| **Memo** | : | ExxonMobil HPV |
| | | |
| **Printing date** | : | 19.04.2005 |
| **Revision date** | : | |
| **Date of last update** | : | 19.04.2005 |
| | | |
| **Number of pages** | : | 30 |
| | | |
| **Chapter (profile)** | : | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile)** | : | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile)** | : | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

### 1.0.1 APPLICANT AND COMPANY INFORMATION

### 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

### 1.0.3 IDENTITY OF RECIPIENTS

### 1.0.4 DETAILS ON CATEGORY/TEMPLATE

**Comment** : This chemical is part of the alkyl acetates category.

**Remark** : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH3COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

### 1.1.0 SUBSTANCE IDENTIFICATION

### 1.1.1 GENERAL SUBSTANCE INFORMATION

### 1.1.2 SPECTRA

### 1.2 SYNONYMS AND TRADENAMES

**C11-C14 branched alkyl acetate ester**

18.12.2000

**Exxate 1300**

07.06.2004

**oxo-tridecyl acetate**

07.06.2004

### 1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

## 2.1 MELTING POINT

| | | |
|---|---|---|
| **Value** | : | = -2 °C |
| **Sublimation** | : | |
| **Method** | : | other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04 |
| **Year** | : | 1999 |
| **GLP** | : | no |
| **Test substance** | : | other TS: C13 methyl-branched alkyl acetate ester |
| **Method** | : | Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle.<br><br>Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.<br><br>The Gold and Ogle Method simply uses the formula<br>Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. |
| **Remark** | : | EPIWIN is used and advocated by the USEPA for chemical property estimation. |
| **Test substance** | : | C13 methyl-branched alkyl acetate ester |
| **Reliability** | : | (2) valid with restrictions<br>The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured. |
| **Flag** | : | Critical study for SIDS endpoint |

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## 2.2 BOILING POINT

| | | |
|---|---|---|
| **Value** | : | = 240 - 285 °C at 1013 hPa |
| **Decomposition** | : | |
| **Method** | : | other: ASTM D1078 Mod |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |
| **Reliability** | : | (4) not assignable<br>This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality. |
| **Flag** | : | Critical study for SIDS endpoint |

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## 2.3 DENSITY

| | | |
|---|---|---|
| **Type** | : | relative density |
| **Value** | : | = .87 at 20 °C |
| **Method** | : | other: ASTM D891 |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |

| | | |
|---|---|---|
| **Reliability** | : | (4) not assignable<br>This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

| | | |
|---|---|---|
| **Value** | : | = .013 hPa at 25 °C |
| **Decomposition** | : | |
| **Method** | : | other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04 |
| **Year** | : | 1999 |
| **GLP** | : | no |
| **Test substance** | : | other TS: C13 methyl-branched alkyl acetate ester |
| **Test condition** | : | Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. |
| **Test substance** | : | C13 methyl-branched alkyl acetate ester |
| **Reliability** | : | (2) valid with restrictions<br>The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.5 PARTITION COEFFICIENT

| | | |
|---|---|---|
| **Partition coefficient** | : | octanol-water |
| **Log pow** | : | = 6.05 at 25 °C |
| **pH value** | : | |
| **Method** | : | other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04 |
| **Year** | : | 1999 |
| **GLP** | : | no |
| **Test substance** | : | other TS: C13 methyl-branched alkyl acetate ester |
| **Test condition** | : | Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92. |
| **Test substance** | : | C13 methyl-branched alkyl acetate ester |
| **Reliability** | : | (2) valid with restrictions<br>The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = .2 mg/l at 25 °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04 |
| **Year** | : | 1999 |
| **GLP** | : | no |
| **Test substance** | : | other TS: C13 methyl-branched alkyl acetate ester |
| **Test condition** | : | Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995. |
| **Test substance** | : | C13 methyl-branched alkyl acetate ester |
| **Reliability** | : | (2) valid with restrictions<br>The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

### 2.13 VISCOSITY

## 2.14 ADDITIONAL REMARKS

### 3.1.1 PHOTODEGRADATION

| | | |
|---|---|---|
| **Type** | : | water |
| **Light source** | : | Sun light |
| **Light spectrum** | : | nm |
| **Relative intensity** | : | based on intensity of sunlight |
| **Deg. product** | : | |
| **Method** | : | other (calculated): Technical Discussion |
| **Year** | : | |
| **GLP** | : | no |
| **Test substance** | : | other TS: C13 methyl-branched alkyl acetate ester |
| **Remark** | : | These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation. |
| **Result** | : | Photolysis as a Function of Molecular Structure |

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

**Test substance** : C13 methyl-branched alkyl acetate ester
**Flag** : Critical study for SIDS endpoint
19.04.2005

**Type** : air
**Light source** :
**Light spectrum** : nm
**Relative intensity** : based on intensity of sunlight
**INDIRECT PHOTOLYSIS**
**Sensitizer** : OH
**Conc. of sensitizer** : 1500000 molecule/cm³
**Rate constant** : = .000000000000186925 cm³/(molecule*sec)
**Degradation** : % after
**Deg. product** :
**Method** : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
**Year** : 1999
**GLP** : no
**Test substance** : other TS: C13 methyl-branched alkyl acetate ester

**Result** : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

| Calculated* half-life (hrs) | OH- Rate Constant (cm3/molecule-sec) |
|---|---|
| 6.9 | 18.69 E-12 |

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

**Test condition** : Indirect photodegradation, or atmospheric oxidation potential, is based on

the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

**Test substance** : C13 methyl-branched alkyl acetate ester
**Reliability** : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
**Flag** : Critical study for SIDS endpoint
19.04.2005 (12)

### 3.1.2 STABILITY IN WATER

### 3.1.3 STABILITY IN SOIL

### 3.2.1 MONITORING DATA

### 3.2.2 FIELD STUDIES

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

### 3.3.2 DISTRIBUTION

**Media** : air - biota - sediment(s) - soil - water
**Method** : Calculation according Mackay, Level I
**Year** : 1998

**Method** : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 242.41 g/mol
Water solubility = 0.2 mg/L
Vapour pressure = 1.33 Pa
log Kow = 6.05
Melting point = -2 deg C

**Result** : Air- 24.2%
Water- 0.07%
Soil- 74.0%
Sediment - 1.6%
Suspended Sed - 0.05%

Biota - <0.01%

**Test substance** : C13 methyl-branched alkyl acetate ester
**Reliability** : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
**Flag** : Critical study for SIDS endpoint
19.04.2005 (17)

## 3.4 MODE OF DEGRADATION IN ACTUAL USE

## 3.5 BIODEGRADATION

**Type** : aerobic
**Inoculum** : other: acclimated inoculum
**Contact time** : 28 day(s)
**Degradation** : = 31 (±) % after 28 day(s)
**Result** :
**Deg. product** :
**Method** : other: USEPA EPA 560/6-83-003, CG-2000 Aerobic Aquatic Biodegradation Test
**Year** : 1982
**GLP** : yes
**Test substance** : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

**Result** : By day 28, 31% degradation of the test material was observed. The half-life, and 10% biodegradation achievement periods were not reported. The positive control (phthalic acid) degraded by 43.8% by day 28, with a TOC removal of 100.7%. TOC was not measured for the test material. The negative control, HgCl2, showed no activity. Biodegradation was based on CO2 evolution. No excursions from the protocol were noted.

**Test condition** : The inoculum was acclimated to the test substance for 14 days prior to study initiation. The media consisted of mineral salt solutions, pond sediment, activated sludge, distilled water, and small amounts (10ul) of test substance. The media was mixed and placed on a gyrorotatory shaker in the dark for 13 days. After settling overnight the supernatant was pour off and was used as the inoculum for the test phase.

The test system utilized 2.0L Glenhill flasks as test vessels. Approximately 13.0 mg (9.6 mg carbon) of test substance was added to 900ml of glass distilled water. Additionally, 100ml of acclimated media and 1ml of mineral salts were added. The flasks were sealed and placed on a gyrorotatory shaker in the dark. Three replicates of the test substance were evaluated. Twice a week, the flasks were monitored for spent NaOH and titrated for carbon dioxide (CO2). Total Organic Carbon (TOC) was measured at initiation and termination in the controls.

A positive and negative control were tested consisting of Phthalic acid (100ml at 103.8mg/L) and HgCl2 (10 ml at 51g/L) respectively, along with three blanks.

Test temperature ranged from 21.5 to 25.0 Deg C.

**Reliability** : (2) valid with restrictions
TOC values not measured on test treatments only controls. No replicate values reported (mean values only).
**Flag** : Critical study for SIDS endpoint
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## 3.6 BOD5, COD OR BOD5/COD RATIO

## 3.7 BIOACCUMULATION

| | | |
|---|---|---|
| **Species** | : | other: see remark |
| **Exposure period** | : | at °C |
| **Concentration** | : | |
| **BCF** | : | = 325 |
| **Elimination** | : | |
| **Method** | : | other: calculation |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | other TS: C13 methyl-branched alkyl acetate ester |
| **Remark** | : | A log BCF of 2.5 (BCF = 325) is calculated. C13 methyl-branched alkyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was CC(=O)OCC(C)CCCCCCC(C)CC |
| **Reliability** | : | (2) valid with restrictions<br>This robust summary has a reliability rating of 2 because the data are calculated and not measured. |
| **Flag** | : | Critical study for SIDS endpoint |

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## 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

| | | |
|---|---|---|
| **Type** | : | flow through |
| **Species** | : | Pimephales promelas (Fish, fresh water) |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | mg/l |
| **LL0** | : | = 5800 measured/nominal |
| **Limit test** | : | no |
| **Analytical monitoring** | : | yes |
| **Method** | : | other: USEPA 40 CFR 792 |
| **Year** | : | 1984 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |

**Result** : 96 hour LL0 = 5800 mg/L based upon nominal loading levels. There was no mortality at saturation.

The amount of TC (total carbon) measured (less the control value) in the exposure solutions was below detection limit.

| Nominal Conc. (% WAF) | Fish Total Mortality (@96 hrs)* |
|---|---|
| Control | 0 |
| 6.25 | 0 |
| 12.5 | 0 |
| 25.0 | 0 |
| 50.0 | 0 |
| 100.0 | 0 |

*20 fish added at test initiation
The analytical method measured Total Carbon (TC). TC was monitored in exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TC for each level tested. No significantly high or low levels were seen.

**Test condition** : A stock water accommodated fraction (WAF) was prepared by adding the test substance to laboratory blend water at a ratio of 1:150. The solution was stirred for 72 hours and the 100% WAF used for testing. The WAF was administered to the test chambers via a diluter system. The diluter system comprised of glass, stainless-steel with no plasticized materials. The diluter prepared the following test treatment levels: control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF. The test chambers were 15L glass tanks containing 14L of solution. Two replicates with ten fish each were tested per treatment level.
Test temperature was 21.78 +/- 0.15 Deg C. Lighting was gradual on and off with 16 hours dark and 8 hour light with an intensity of 77 to 79 ft candles.
Dilution water hardness was 158 mg/L as CaCO3.
The pH ranged from 7.6 to 8.0. Dissolved Oxygen ranged from 7.7 to 8.6 mg/L.
Fish were supplied by in-house laboratory; age = 25 weeks; mean wt.=0.276g; mean total length=2.5cm; test loading=0.023g of fish/L per 24 hour period.

| | | |
|---|---|---|
| **Conclusion** | : | The test material is considered non-toxic at its level of water solubility. |
| **Reliability** | : | (1) valid without restriction |
| **Flag** | : | Critical study for SIDS endpoint |

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## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

| | | |
|---|---|---|
| **Type** | : | static |
| **Species** | : | Daphnia magna (Crustacea) |
| **Exposure period** | : | 48 hour(s) |
| **Unit** | : | mg/l |
| **EL0** | : | = 5829 measured/nominal |
| **Limit Test** | : | no |
| **Analytical monitoring** | : | yes |
| **Method** | : | other: USEPA 560/6-82 |
| **Year** | : | 1984 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |

**Result** : 48 hour EL0 = 5829 mg/L based upon nominal loading levels. There was no immobility at saturation.

| Nominal. Conc. (% WAF) | Daphnia Total Immobility (@48 hrs)* |
|---|---|
| Control | 0 |
| 6.25 | 0 |
| 12.5 | 0 |
| 25.0 | 0 |
| 50.0 | 0 |
| 100.0 | 0 |

*40 Daphids total added at test initiation.
Mortality is defined as immobilized.
Some daphnids observed swimming on the surface in all treatment levels.

Three trials of the study were performed to confirm study results. Trials 2 and 3 exhibited no toxicity (trial 1 was not reported). The third trial is documented here.
Analytical method used was Total Carbon (TC). The measured TC values (less the controls) were within the variability of the analytical method. TC was monitored in exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TC for each level tested. No significantly high or low levels were seen.

**Test condition** : A water accomodated fraction (WAF) was prepared as a stock solution and then diluted to prepare the individual treatment levels. The WAF was prepared by adding 16.75ml of the test substance to 2.5L of laboratory dilution water in a glass carboy and mixed with a magnetic stir plate and bar. After mixing for 72 hours, the 100% WAF was drawn out through a sampling tube.
Test vessels were 400ml glass beakers filled with 250ml of solution and covered. Four replicates were prepared for each treatment. Each replicate contained 10 organisms.
Nominal treatment levels were; control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF.
Test temperature was 20.92 Deg C. Lighting measured 78 to 85 ft. candles with 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 8.3 to 9.5mg/L. The pH ranged from 8.2 to 8.5 units.

Organisms were supplied by in-house cultures; age = <24 hours old.
Parents age = 13 days old.

| | | |
|---|---|---|
| **Reliability** | : | (1) valid without restriction |
| **Flag** | : | Critical study for SIDS endpoint |

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## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

| | | |
|---|---|---|
| **Species** | : | Selenastrum capricornutum (Algae) |
| **Endpoint** | : | growth rate |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | mg/l |
| **Limit test** | : | no |
| **Analytical monitoring** | : | yes |
| **Method** | : | other: USEPA, EPA 560/6-83-002 |
| **Year** | : | 1983 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |

**Result** :

96 hour EL0b: = 5829 mg/L based upon calculated laoding level.
96 hour EL0gr: = 5829 mg/L based upon calculated loading level.
There was no inhibition at saturation.

NOELRb = 5829 mg/L based upon nominal loading levels.
NOELRgr= 5829 mg/L based upon nominal loading levels.

No Inhibition of Algal growth was observed at the highest treatment level 100% WAF (0.873 ppm Carbon)

| Nominal Conc. (%WAF) | Mean Cell Conc. - 96 hr (cells/ml) |
|---|---|
| Control | 5.2x10(6) |
| 6.25 | 4.4 x10(6) |
| 12.5 | 4.6 x10(6) |
| 25.0 | 4.1 x10(6) |
| 50.0 | 5.3 x10(6) |
| 100.0 | 5.2 x10(6) |

Analytical method used was Total Carbon (TC). Measured TC values are based upon Day 0 samples less the control value on day 0 of the study. TC was monitored in exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TC for each level tested. No significantly high or low levels were seen.

No excursions from the protocol were noted.

**Test condition** : A Water Accommodated Fraction (WAF) stock solution was prepared by adding 6.7ml of test substance to 1L of algal nutrient media (AAP) in a 2L flask and mixed slowly for 72 hours. After mixing, the solution was transferred to a separatory funnel and allowed to settle for one hour. After settling, the solution was removed from the bottom and used as the 100% WAF. Individual treatments were prepared by diluting the 100% WAF with algal nutrient media. The test treatments were divided into 4 replicates. Three replicate were inoculated with algae at 2.0 x 104. The remaining replicate served as a blank. Treatment replicates were 125 ml erlenmeyer flasks containing 50 ml of solution. Flasks were placed on a shaker table during the study at ~100 rpm.
The test treatment concentrations were; control, 6.25, 12.5, 25, 50 and 100% WAF which measured (less the control value) na, 0, 0.058, 0.219, 0.492, and 0.873ppm of TC.

Test temperature was 23.89 Deg. C. Lighting was continuous at 400 ft candles. The pH was 7.5 at test initiation and ranged from 7.3 to 7.4 at test termination.

| | | |
|---|---|---|
| **Reliability** | : | (1) valid without restriction |
| **Flag** | : | Critical study for SIDS endpoint |

19.04.2005 (9)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

### 5.1.1 ACUTE ORAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | other: Limit |
| **Value** | : | > 5000 mg/kg bw |
| **Species** | : | rat |
| **Strain** | : | Sprague-Dawley |
| **Sex** | : | male/female |
| **Number of animals** | : | 5 |
| **Vehicle** | : | other: none |
| **Doses** | : | 5.721 ml/kg |
| **Method** | : | other: Experimental |
| **Year** | : | 1983 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |
| **Remark** | : | Route of Administration: oral gavage. Number of animals per dose per sex = 5. Single (18-hr fasted) dose of 5.721 ml/kg (1.1-1.9 ml). Post dose observation period of 14 days.<br><br>There were no deaths during this study. Nine of 10 animals showed staining in the ano-genital area on Days 1 and 2, and for 1 animal on Day 3. Soft stool was noted for 1 animal at 6 Hrs PD and white gelatinous material on the penis was noted for 1 animal on Day 1. There were no observable abnormalities noted after the Day 3 observations. All animals except one showed an increase over pre-dose weights except one animal that appeared to have had an incorrect pre-dose weight recorded. Six of 10 animals showed no observable abnormalities during postmortem examination. Four animals showed lung discoloration typical of findings resulting from carbon dioxide asphyxiation. |
| **Conclusion** | : | C11-C14 branched alkyl acetate ester elicited minimal signs of acute systemic toxicity when administered orally. Signs of slight toxicity (staining of the fur and soft stool) were limited to the first 3 days. |
| **Reliability** | : | (1) valid without restriction<br>No Circumstances occurred that would have affected the quality or integrity of the data. |
| **Flag** | : | Critical study for SIDS endpoint |

19.04.2005 (7)

| | | |
|---|---|---|
| **Type** | : | other: Repeated-Dose Probe |
| **Value** | : | > 3000 mg/kg bw |
| **Species** | : | rat |
| **Strain** | : | Sprague-Dawley |
| **Sex** | : | male/female |
| **Number of animals** | : | 4 |
| **Vehicle** | : | other: none |
| **Doses** | : | 0, 0.1, 0.5, 1.0, or 3.0 g/kg |
| **Method** | : | other: Experimental |
| **Year** | : | 1985 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |
| **Remark** | : | Route of Administration: oral gavage. Number of animals per dose per sex = 4. Doses / time: 0, 0.1, 0.5, 1.0, or 3.0 g/kg / Once daily for a total of |

9 doses. Vol. Admin.: < or = 3.333 ml/kg. Post dose observation period of 11 days.

One control animal was euthanized on Day 7 due to a moribund condition following a caging accident. All other animals survived to study termination and exhibited increases in body weight. In-life clinical observations showed no observable abnormalities throughout the study period for the surviving control animals and the majority of those dosed with 0.1, 0.5, or 1.0 g/day. The animals dosed with 3.0 g/day showed scattered incidences of wet rales, protruding penis, urinary and fecal staining, and soft stool; for the majority of the test period they showed no observable abnormalities. As a group, only the 0.1 males showed decreases in mean hematocrit and hemoglobin compared to controls (values for 2 animals were significantly lower than all other animals). Females showed significant decreases in mean red blood cell count, hematocrit, and hemaglobin values compared to controls. Gross postmortem examination showed dilated renal pelvis for 1 control and 1 animal of the 1.0 g/day dose group. A large discolored ovary was observed in a 0.1 g/day animal and a thymic discoloration was seen in a 0.5 g/day animal. Two animals at the 3.0 g/day dose level showed staining of the ano-genital area.

**Conclusion** : C11-C14 branched alkyl acetate ester elicited minimal signs of acute systemic toxicity when administered once daily for a total of 9 doses by oral gavage.

**Reliability** : (1) valid without restriction
No Circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint
19.04.2005 (3)

### 5.1.2 ACUTE INHALATION TOXICITY

### 5.1.3 ACUTE DERMAL TOXICITY

**Type** : other: Limit
**Value** : > 3160 mg/kg bw
**Species** : rabbit
**Strain** : New Zealand white
**Sex** : male/female
**Number of animals** : 3
**Vehicle** : other: none
**Doses** : 3160 mg/kg bw
**Method** : other: Experimental (Non-regulatory)
**Year** : 1984
**GLP** : yes
**Test substance** : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

**Remark** : Route of Administration: dermal application. Number of animals per dose per sex = 3. Single application / 24-hour occlusive patch of 3160 mg/kg. Post dose observation period of 14 days.

There were no overt signs of systemic toxicity. Five of 6 rabbits showed slight body weight decreases at Day 7; only 2 animals continued to have decreased body weight at 14 days. Slight dermal irritation persisted in 4 of 6 test animals through termination of the study. In general, dermal responses were considered minimal and transient in nature. At post mortem examination, 3 of 6 animals showed no observable abnormalities. Liver and salivary gland discoloration was observed in one animal; kidney

discoloration and spleen enlargement in another; and alopecia in the third animal.

**Conclusion** : C11-C14 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.

**Reliability** : (1) valid without restriction
No Circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint

19.04.2005 (2)

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.2.1 SKIN IRRITATION

**Species** : rabbit
**Concentration** : .5 other: ml
**Exposure** : Semiocclusive
**Exposure time** : 4 hour(s)
**Number of animals** : 6
**Vehicle** :
**PDII** : .67
**Result** :
**Classification** :
**Method** : EPA OTS 798.4470
**Year** : 1983
**GLP** : yes
**Test substance** : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

**Remark** : Route of Administration: dermal application. Number of animals per dose per sex = 3. Single application / 4-hour semi-occlusive patch of 0.5 ml. Post dose observation period 1, 24, 48, and 72 hours and Day 7.

All animals survived to study termination, were free of clinical signs, and 5 of 6 animals displayed an increase in body weight during the test period. All animals showed erythema in the first 72 hours. The mean score for erythema was 0.67. One of 6 animals showed very slight erythema at the day 7 observation. The study was terminated on Day 7.

**Result** : mild dermal irritant to rabbit skin.

**Conclusion** : C11-C14 branched alkyl acetate ester is a mild dermal irritant to rabbit skin.

**Reliability** : (1) valid without restriction
No Circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint

19.04.2005 (5)

### 5.2.2 EYE IRRITATION

**Species** : rabbit
**Concentration** : 100 %
**Dose** : .1 ml
**Exposure time** :
**Comment** :
**Number of animals** : 3
**Vehicle** : none
**Result** :
**Classification** :

| | | |
|---|---|---|
| **Method** | : | EPA OTS 798.4500 |
| **Year** | : | 1983 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |
| **Remark** | : | Draize Ocular Irritation on male and female New Zealand White rabbits. Number of animals per dose per sex = 3. Ocular instillation into the conjunctival sac of right eye using untreated left eye as control. Single instillation of neat material. Post dose observation period 1, 4, 24, 48 and 72 hours postinstillation and once/day on days 4 and 7. Vehicle: none.<br><br>Ocular irritation was most prominent at the 1-hour observation when the total Draize scores ranged from 0 to 6 (Maximum possible score = 110). Irritation was confined to the conjunctivae and generally consisted of redness, chemosis and discharge. Corneal ulceration was noted and confirmed using fluorescein stain in one animal at the 24-hour observation. The signs of eye irritation completely subsided in all animals by the day 7 evaluation. |
| **Result** | : | Minimal Irritation |
| **Conclusion** | : | C11-C14 branched alkyl acetate ester was a mild reversible irritant. |
| **Reliability** | : | (1) valid without restriction<br>No circumstances occurred that would have affected the quality or integrity of the data. |
| **Flag** | : | Critical study for SIDS endpoint |

19.04.2005 (1)

## 5.3 SENSITIZATION

## 5.4 REPEATED DOSE TOXICITY

| | | |
|---|---|---|
| **Type** | : | |
| **Species** | : | rat |
| **Sex** | : | male/female |
| **Strain** | : | Sprague-Dawley |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | 90 days |
| **Frequency of treatm.** | : | once/day |
| **Post exposure period** | : | |
| **Doses** | : | 0, 0.1, 0.5, and 1.0 g/kg/day |
| **Control group** | : | yes |
| **NOAEL** | : | = 1000 mg/kg |
| **Method** | : | EPA OTS 798.2650 |
| **Year** | : | 1985 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |
| **Remark** | : | 13-Week Repeated Dose Oral Toxicity on 20 male & female rats. Volume: < or = 1.111 ml/kg (controls received a dose of water volumetrically comparable to the dosage administered to the high dose group, 1.111 ml/kg). Vehicle: none.<br><br>Clinical laboratory studies (hematology and serum chemistry) were performed pretest on 5 males and 5 females (non-study animals), on 5 animals/sex/dose after 45 days (interim sacrifice), and all animals at study termination. Blood samples were collected from the abdominal aortas following an overnight fast. At 45 days, a complete necropsy was |

performed and livers were collected, weighed and preserved. After 13 weeks, all surviving animals were weighed, anesthetized and sacrificed by exsanguination. Complete necropsies were performed.

**Result** : Liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects.

**Conclusion** : Oral administration of C11-C14 branched alkyl acetate ester daily, 5 days/week for 13 weeks, to rats produced minimal signs of systemic toxicity. There was no treatment-related mortality. The in-life clinical observations were primarily oral and dermal irritation (no clear dose-response). Weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels. At the terminal sacrifice, glucose values for the 0.5, and 1.0 g/kg/day males were lower than controls and the total protein values for the 1.0 g/kg/day females were higher than controls. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and not indicative of toxic effects. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy in the mid- and high-dose male rats that were consistent with alpha-2u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix/corpus of the uterus, and vagina), showed normal morphology. The lowest observable effect level was 500 mg/kg. No effects were observed at 100 mg/kg.

**Reliability** : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint
19.04.2005 (6)

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : other: Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)

**System of testing** : Bacterial

**Test concentration** : 156, 312.5, 625, 1250, 2500, 5000, and 10000 µg/plate (312.5 repeat assay only; 5000 and 10,000 initial assay only)

**Cycotoxic concentr.** :

**Metabolic activation** : with

**Result** : negative

**Method** : other: FIFRA 84-2

**Year** : 1994

**GLP** : yes

**Test substance** : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

**Remark** : Species/Strain: S. typhimurium / TA98, TA100, TA1535, tA1537, TA1538. Species/cell type: Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9). Vehicle: DMSO.

**Result** : C11-C14 branched alkyl acetate ester, did not induce significant increases in revertant colonies (> 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either

a reduction in the number of revertant colonies or a reduction in the background lawn, was not observed. Test substance beading was observed for all tester strains, both with and without metabolic activation at 1250 through 10000 µg/plate. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

**Test condition** : There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 156, 312.5, 625, 1250, 2500, 5000, and 10000 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 ºC for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

**Conclusion** : C11-C14 branched alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested and was not toxic in any strain tested under the conditions of this study.

**Reliability** : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint
19.04.2005 (15)

## 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : other: In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method
**Species** : mouse
**Sex** : male/female
**Strain** : other: Crl:CD-1 (VAF/Plus)
**Route of admin.** : gavage
**Exposure period** : 24, 48 and 72 hours
**Doses** : 0.45, 0.90, and 1.80 grams/kg / Single dose
**Result** : negative
**Method** : EPA OTS 798.5395
**Year** : 1994
**GLP** : yes
**Test substance** : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

**Remark** : The vehicle used was corn oil. Cyclophosphamide (40 mg/kg) in reagent grade water by oral gavage was used as a positive control. Number of animals per sex per dose = 5.

The test substance and the vehicle were administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with Cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were

removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for presence of micronuclei (1000 polychromatic erythrocytes/animal were evaluated).

The test material is considered to be toxic to bone marrow in CD-1 mice based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time.

**Result** : A dose-related decrease in the percentage of polychromatic erythrocytes was observed for the female 48-hour sampling time (regression coefficient $p<0.01$). However, none of the dose groups were statistically different from the control. The positive control (40 mg/kg cyclophosphamide) induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes ($p<0.01$) which indicates that the positive control is clastogenic and is responding in an appropriate manner. Vehicle carrier control values for the mean percent of polychromatic erythrocytes and for the mean percent of micronucleated polychromatic erythrocytes responded in an appropriate manner.

**Conclusion** : C11-C14 branched alkyl acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.

**Reliability** : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint
19.04.2005 (14)

## 5.7 CARCINOGENICITY

## 5.8.1 TOXICITY TO FERTILITY

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | Sprague-Dawley |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | Gravid Day 6-15 |
| **Frequency of treatm.** | : | single dose daily |
| **Duration of test** | : | Gravid Day 20 |
| **Doses** | : | 0, 500, 1300, and 2500 mg/kg |
| **Control group** | : | other: Sham-Treated with distilled water at 2.5 g/kg |
| **NOAEL maternal tox.** | : | = 500 mg/kg bw |
| **NOAEL teratogen.** | : | = 2500 mg/kg bw |
| **other: NOEL Maternal** | : | = 500 mg/kg bw |
| **other: NOEL Pup** | : | = 2500 - mg/kg bw |
| **Method** | : | EPA OTS 798.4900 |
| **Year** | : | 1985 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13) |

**Remark** : Developmental Toxicity with 22 mated females per dose. Vehicle: none.

Statistical Methods: Maternal body weight, body weight change, food

consumption, uterine data (i.e., corpora lutea, implants, resorptions), and malformation data were analyzed with Bartlett's test of homogeneity of variance to determine if groups had equivalent variances at the 15 level of significance. If not significantly different, groups were compared using a one-way standard analysis of variance (ANOVA). If significant differences among means were detected, Duncan's test was used to determine the treated group that differed from control. Fetal weights and crown-rump lengths were analyzed using individual fetal values by a standard nested analysis of variance with values nested within dams and dams nested within groups. If differences within groups were indicated, the least-significant-difference technique was used to determine the group(s) that differed from control. If the groups did not have equivalent variances at the 1% level, then a Kruskal-Wallis test (nonparametric) was used to assess differences in group means. If the means were different, a rank sum comparison was used to determine the treatment group that differed from control.

**Result** : There were no statistically significant deleterious effects on survival, fetal body weight, crown-rump length or malformations at any dose.

**Conclusion** : C11-C14 branched alkyl acetate ester was administered at 0, 500, 1300, and 2500 mg/kg on gestation days 6-15 in a developmental toxicity study in rats. Maternal toxicity was seen at the 1300 and 2500 mg/kg doses as evidenced by decreases in body weight. There were no statistically significant deleterious effects on fetal survival, body weight, or crown-rump length and no evidence of treatment-related malformations.

**Reliability** : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

**Flag** : Critical study for SIDS endpoint
19.04.2005 (4)

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

### 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

## 6.1 ANALYTICAL METHODS

## 6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bio/dynamics Inc, East Millstone, NJ; Project # 330613.

(2) Bio/dynamics Inc., East Millstone, NJ, Acute Dermal Toxicity Study in the Rabbit; Project # 330606.

(3) Bio/dynamics Inc., East Millstone, NJ, Oral Gavage Probe Study in the Rat; Project # 252171.

(4) Bio/dynamics Inc., East Millstone, NJ, Oral Teratology Study in Rats; Project # 352134.

(5) Bio/dynamics Inc., East Millstone, NJ, Primary Dermal Irritation Study in the Rabbit; Project # 330604.

(6) Bio/dynamics Inc., East Millstone, NJ, Subchronic Oral Gavage Study in Rats; Project # 252170.

(7) Bio/dynamics, East Millstone, NJ, Acute Oral Toxicity Study in the Rat; Project # 330601.

(8) BioDynamics Inc. 1985. A Flow-Through Acute Fish Toxicity Test. Study #252141.

(9) BioDynamics, Inc. 1985. An Acute Algal Toxicity Test. Study #252159.

(10) BioDynamics, Inc. 1985. Ultimate Biodegradability. Study # 252189.

(11) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(12) EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(13) Exxon Biomedical Sciences, Inc. 1985. An Acute Static Daphnia Toxicity Test. Study # 252142A.

(14) Exxon Biomedical Sciences, Inc., East Millstone, NJ, In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method, Project # 168930.

(15) Exxon Biomedical Sciences, Inc., East Millstone, NJ, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay; Study # 168925.

(16) ExxonMobil Chemical Company (2003). Exxate 1300 Data Sheet.

(17) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

## 10.1 END POINT SUMMARY

## 10.2 HAZARD SUMMARY

## 10.3 RISK ASSESSMENT